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Incorporation of Chemical Reactions Into Building-scale Flow

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Disclaimer

INCORPORATION OF CHEMICAL REACTIONS INTO BUILDING-SCALE FLOW

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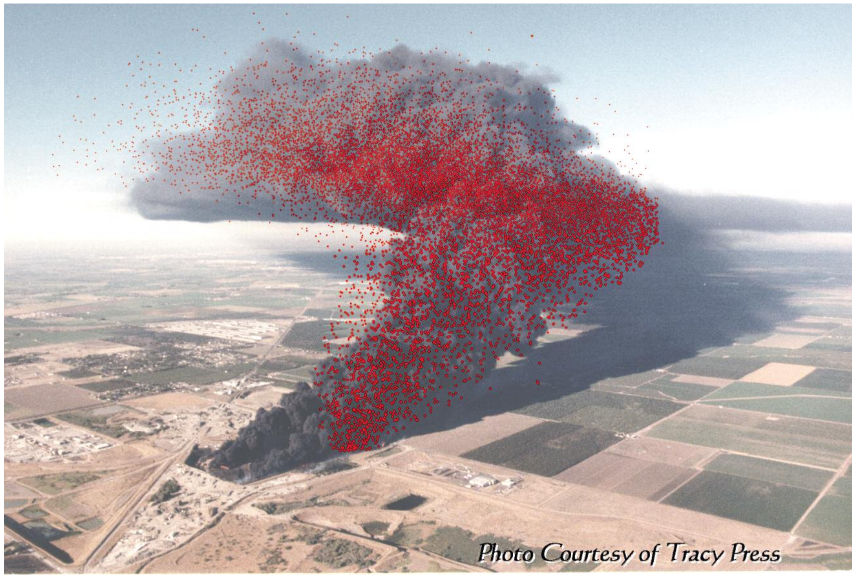
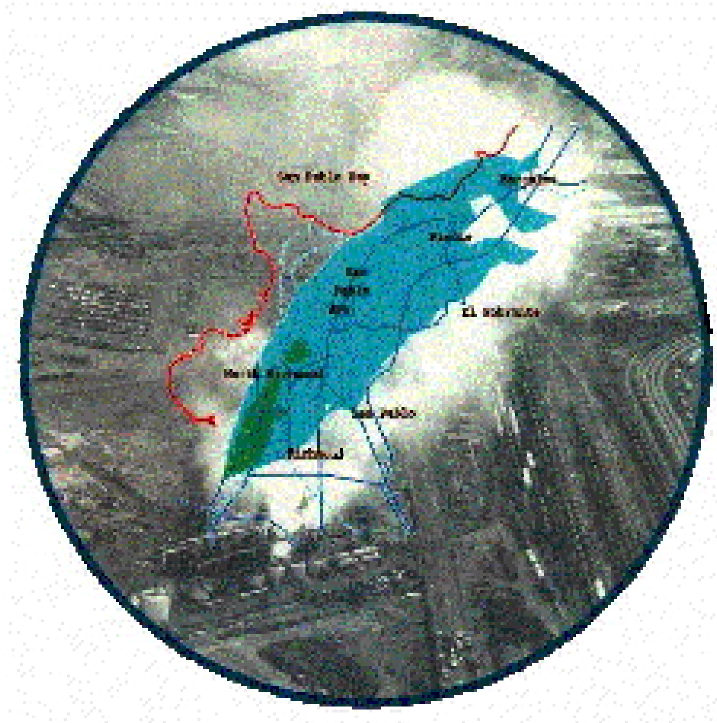
MANY ATMOSPHERIC RELEASES INVOLVE CHEMICALLY REACTING COMPOUNDS



1998 TRACY TIRE DUMP FIRE

RELEASES FROM CHEMICAL PLANTS



1993 RICHMOND CHEMICAL SPILL

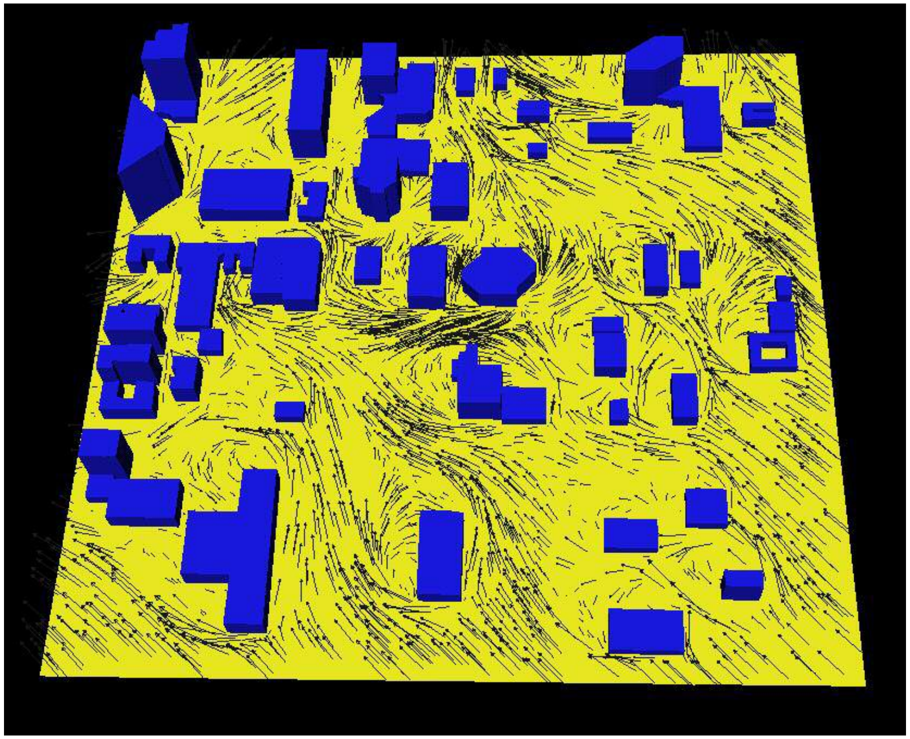
Need for Chemistry and Dispersion

- Reactions may reduce or increase the threat posed by an atmospheric release
- Source detection depends on knowing what to look for, where
- More accurate source terms for incorporation into larger-scale dispersion models
- Local reactant dispersion patterns resolvable with high-resolution simulations

Computational Fluid Dynamics (CFD) Model

FEM3MP

- **Finite Element Method, 3D, Massively Parallel**
- **Subgrid Scale Model options (e.g., RANS, LES)**
- **Basic Aerosol Model**
- **Basic Surface Energy Budget**
- **Currently being upgraded to include AMR (Kosovic), two-way integration with larger-scale models**



Above:
- **Domain width: 1 km**
- **Building size: 50 m**
- **Finest grid spacing: 1 m**
- **Velocity shown: 1 m/sec**

Chemistry Model

SMV Gear II Solver
by Mark Jacobson

- Sparse Matrix, Vectorized, Gear-type integrator for first-order coupled ODE's
- Provided to us by Philip Cameron-Smith and Peter Connell (LLNL) from their global chemistry code, IMPACT

Mechanism

- List of ~30 Species
- Reactions of type
  $A + B \rightarrow C + D$
- Rate constants and activation energies
  Rate =
  $k * \exp(-E_a / RT) * [A] * [B]$

CONSTRUCTION

Assembly

- SMV Gear routines incorporated into one module of FEM3MP
- Mechanism text translated to code with scripts written by Peter Connell (LLNL)
- Mechanism code incorporated during compilation

Testing

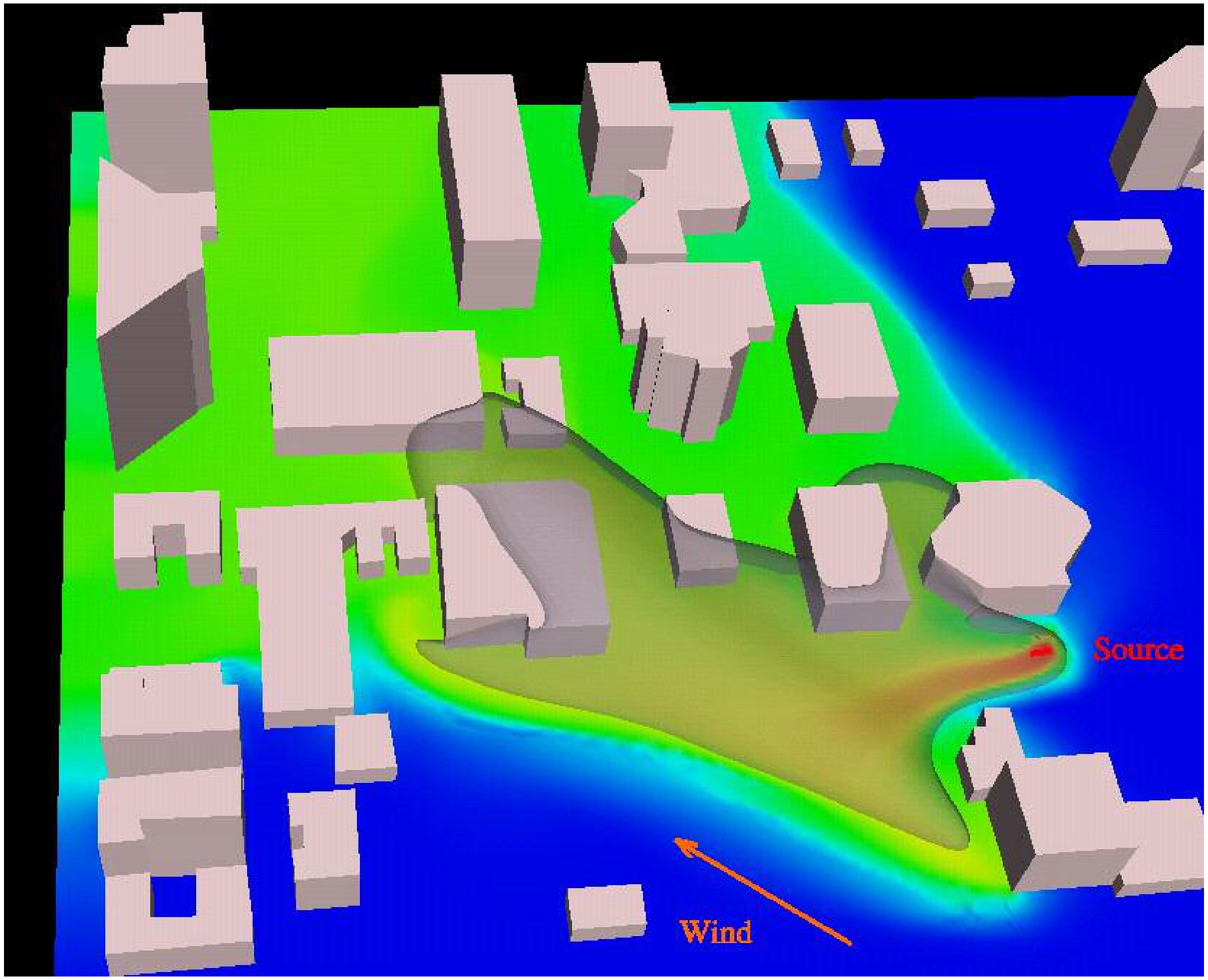
- Standalone SMV Gear routines tested against separate box model
- FEM3MP with SMV Gear routines tested with no advection or diffusion, and uniform concentrations
- Concentrations nearly independent of time step: 1 sec, 0.5 sec, 0.25 sec.

Features of Reaction Product Plumes 1

Limited Area of High Product Concentrations

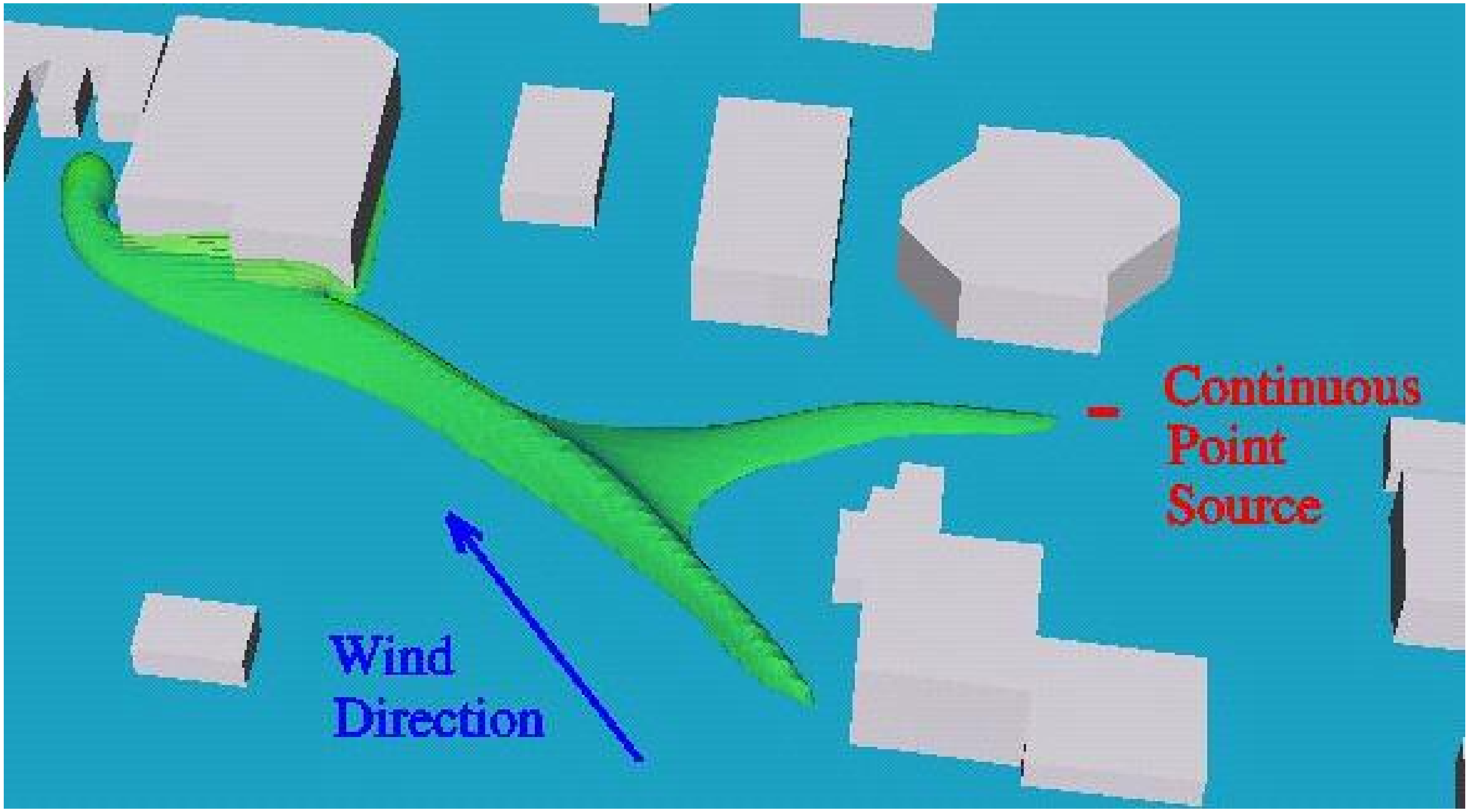
- Ground colored by release material

- Product (grey isosurface) near release only



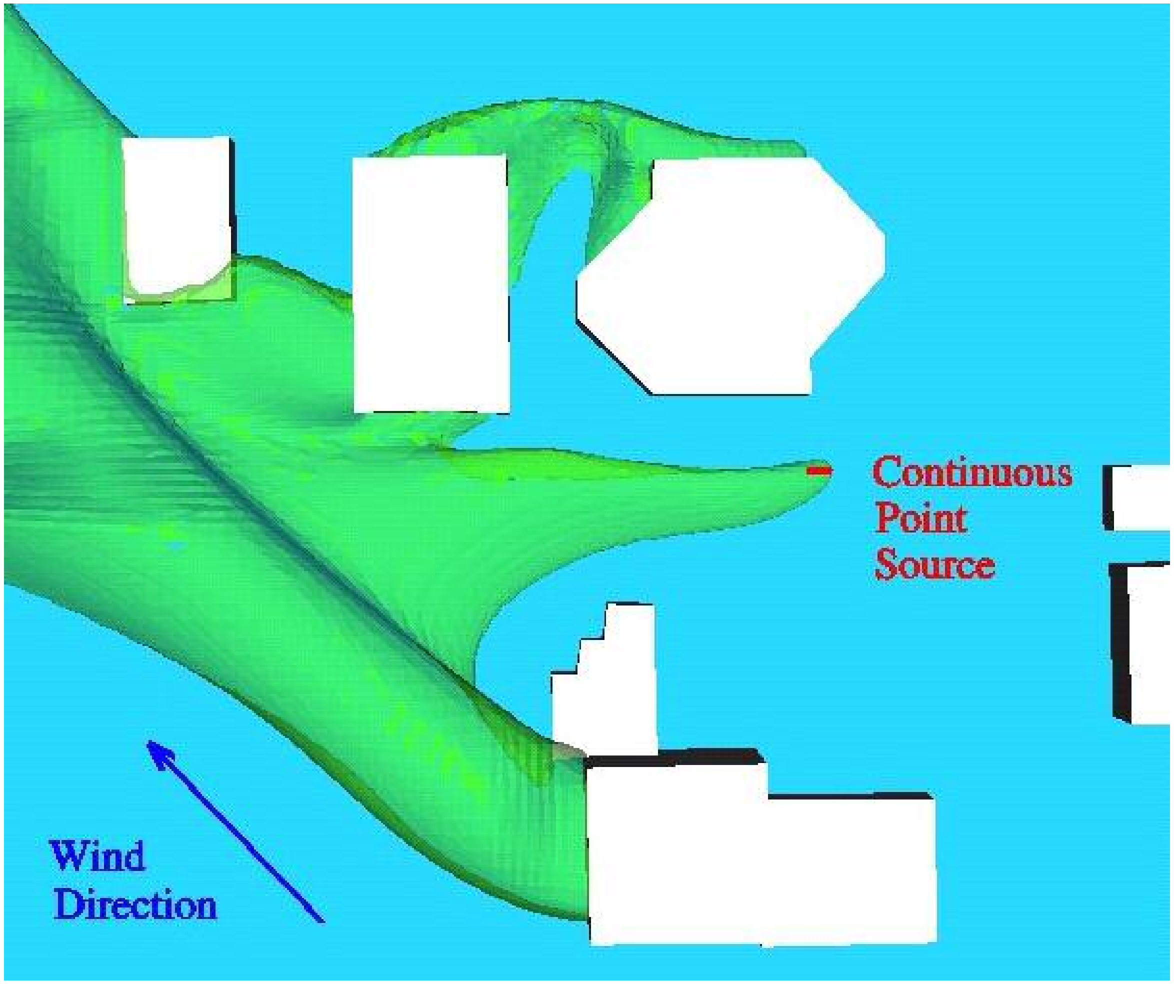
Features of Reaction Product Plumes 2

Maximum product concentration separated from source



Features of Reaction Product Plumes 3

Local “Hot Spots” in Building Wakes



Current and Future Directions

- Include aqueous reactions within and heterogeneous reactions on the surfaces of droplets
- Increase number of mechanisms for common industrial and pollutant compounds
- Integration with larger scale chemistry models